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QUANTUM THEORY OF THE EMISSION PROCESS*,§

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Summary: It is shown, that the emission process of a photon during the transition of an atom between two quantum states can be described in closed form by a superposition of stationary states of the total system, consisting of the atom coupled by the interaction to the system of field oscillators. In this treatment all physical quantities involved remain finite and no improper, quadratically non-integrable functions occur. The theory leads only in first approximation to the expression of the older theory and reveals more details, which become of some importance in the immediate neighborhood of resonance.

1. Introduction: It is well known that the classical expression for the emission of a wave train by an electric oscillation, given by Hertz' solution

$$\vec{Z} = \frac{\vec{Z}}{r} \cdot \exp\left\{i(k_0 - i\gamma)\cdot(r-ct)\right\} \quad , r < ct \qquad (1)$$

has no proper spectrum, i.e., it cannot be represented by an ordinary Fourier integral. The integral, which represents (1) in momentum

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space is essentially a complex integral

$$\vec{Z} = -\frac{\vec{Z}}{\pi r}\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{\exp(-ikct}{\bar{k}-k_0+i\gamma}\,d\bar{k}\int_{-\infty}^{+\infty}\frac{\sin kr}{k-\rho}\,dk \qquad (2)$$

the path of which has to be appropriately chosen. Any complex path of integration implies, however, complex frequencies and therefore, cannot be interpreted in terms of a spectral analysis by means of any spectral apparatus. If we try to interpret (2) along the real axis of k, we are led to define $1/(k-\bar{k})$ by a quadratically non-integrable improper function, the Schwartz' distribution

$$1/(k-\bar{k}) = 2i\pi\delta_+(k-\bar{k}) = i\cdot\pi\delta(k-\bar{k}) + P\,1/(k-\bar{k}) \qquad (3)$$

(P = principal value). The difficulty arising in (2) and (3) derives from the fact that we cannot attribute a finite probability to any configuration of photons of given wavelength k and frequency $\bar{k}$.

We have concluded from this fact, in an earlier paper [1] that only the external parts of (3) can correspond to physical reality, while the parts close to the singularity have to be modified by a more detailed treatment of the involved physical problem.

We shall show, in what follows, that it is sufficient for our purpose, to consider a finite system in which a mechanical oscillator, represented by two states only, is coupled to a finite set of discreet electric dipole vibrations in an appropriately chosen cavity of finite size with perfectly reflecting walls. We neglect, in this treatment, waves of very high frequency, virtual transitions to higher states of the mechanical system and all configurations in which more than one photon are present simultaneously. We suppose that all these omitted configurations do not appreciably influence the emission process, if we restrict ourselves to the weak coupling case only.

2. The coupled system. We shall denote by k_0 the unperturbed frequency of our mechanical oscillator and by c_0 its probability ampli-

tude in the excited state (oscillator excited, no photon present) and by

$$k_1,\ k_2 \ \ldots\ldots\ k_k \ \ldots\ldots$$

$$c_1,\ c_2 \ \ldots\ldots\ c_k \ \ldots\ldots$$

the unperturbed frequencies and probability amplitudes of the field states (oscillator in ground state, one photon present).

Establishing an interaction between the mechanical oscillator and each individual electromagnetic vibration, the unperturbed frequency spectrum of the total system will become shifted and the new frequency spectrum becomes

$$\bar{k}_0,\ \bar{k}_1,\ \bar{k}_2 \ \ldots\ldots\ \bar{k}_k \ \ldots\ldots$$

To each value $\bar{k}_\ell$ belongs a normal vibration of the total system, a collective motion in which, in general, both the mechanical oscillator and all considered electromagnetic vibrations will participate.

The ℓ-th normal vibration will be determined by the set of equations

$$\begin{aligned}
&(k_0-\bar{k}_\ell)\cdot c_0^\ell + \alpha_{01}\cdot c_1^\ell + \alpha_{02}\cdot c_2^\ell + \ldots\ldots = 0\\
&\alpha_{10}\cdot c_0^\ell + (k_1-\bar{k}_\ell)\cdot c_1^\ell = 0\\
&\alpha_{20}\cdot c_0^\ell + (k_2-\bar{k}_\ell)\cdot c_2^\ell = 0\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned} \qquad (4)$$

The α_{ok} and α_{ko} represent the coupling constants (matrix elements) of our system. For the moment they only have to satisfy the requirement of forming a hermitian matrix.

The simple structure of (4) facilitates greatly the discussion. We conclude immediately from (4):

a. The probability amplitudes c_k^ℓ satisfy both the orthogona-

lity relations

$$\sum_K c_K^{\ell *} \cdot c_K^{\ell'} = \delta^{\ell\ell'} \tag{5}$$

and the completeness relations

$$\sum_\ell c_K^{\ell *} \cdot c_{K'}^{\ell} = \delta_{KK'} \tag{6}$$

if these quantities are normalized in the usual way to unity.

b. For the perturbed frequencies $\bar{k}_\ell$ the following relation holds

$$k_k - \bar{k}_\ell \neq 0 \quad \text{for} \quad k = 1, 2 \ldots; \quad \ell = 0, 1 \ldots. \tag{7}$$

According to (7) no crossing of the eigenvalues is possible, whatever may be the strength of the coupling constants. In other words,

$$k_{\ell-1} < k_\ell < k_{\ell+1} \tag{8}$$

3. The initial conditions. We consider, now, the time dependent probability amplitudes

$$C_K^\ell(t) = c_K^\ell \cdot \exp(-i\bar{k}_\ell \cdot ct) \tag{9}$$

Instead of considering the single normal vibrations of the system to which (9) refers, we can consider "wave packets", i.e., superpositions of normal vibrations, to which more envolved time dependence corresponds. This can be done by means of an arbitrary unitary transformation S_r^ℓ,

$$\sum S_r^\ell \cdot C_K^\ell(t) = D_{rK}(t) \tag{10}$$

which describes the time development of the probability amplitude of the k-th state in the r-th "wave packet". Choosing the unitary transformation S_r^ℓ appropriately, we can assure, for t = 0, any given initial configuration.

If we choose, in particular,

$$S_r^\ell = c_r^{\ell *} \tag{11}$$

we find according to (9), (10) and (6)

$$D_{mk}(t) = \sum_\ell c_r^{\ell *} \cdot c_\ell^\ell \cdot \exp(-i\bar{k}_k ct) \tag{12}$$

$$D_{rk}(0) = \delta_{rk} \tag{13}$$

The unitary transformation (11) transforms, therefore, for t = 0, the uncoupled individual vibrations to principal axis.

In particular, $D_{ok}(0) = \delta_{ok}$ describes the state, in which initially only the excited mechanical oscillator is present and no photons exist in the field. $D_{oo}(t)$ describes, therefore, the damping of the excited oscillator state, while

$$D_{ok}(t) \quad , \quad k \neq 0$$

describes the emission of the field.

Expressions (12) can, for r = 0, still be considerably simplified. Replacing in (5) for c_k^ℓ the values which we find from (4),

$$c_k^\ell = \frac{\alpha_{ko}}{\bar{k}_\ell - \bar{k}_k} c_o^\ell \tag{14}$$

we obtain

$$c_o^{\ell *} \cdot c_o^\ell \left\{ 1 + \sum_{r \neq o} \frac{\alpha_{or}\alpha_{ro}}{(\bar{k}_\ell - \bar{k}_r)^2} \right\} = 1$$

or
$$c_o^{\ell *} \cdot c_o^{\ell} = \left\{ 1 + \sum_{r \neq 0} \frac{\alpha_{or}\alpha_{ro}}{\left[\bar{k}_\ell - k_r\right]^2} \right\}^{-1} \tag{15}$$

From (12), with (14) and (15), we find for the quantities in which we are interested

$$D_{oo}(t) = \sum_\ell \left\{ 1 + \sum_{r \neq 0} \frac{\alpha_{or}\alpha_{ro}}{\left[\bar{k}_\ell - k_r\right]^2} \right\}^{-1} \cdot \exp\left(-i\bar{k}_\ell ct\right) \tag{16}$$

$$D_{ok}(t) = \sum_\ell \frac{\alpha_{ko}}{\bar{k}_\ell - k_k} \left\{ 1 + \sum_{r \neq 0} \frac{\alpha_{or}\alpha_{ro}}{\left[\bar{k}_\ell - k_r\right]} \right\}^{-1} \cdot \exp\left(-ik_k \cdot ct\right) \tag{17}$$

being
$$D_{ok}(t) = i \cdot \alpha_{ko} \exp\left(+ik_k \cdot ct\right) \cdot \int_0^t D_{oo}(t) \cdot \exp\left(ik_k \cdot ct\right) c\,dt \tag{18}$$

4. An approximate solution of (16). The relations (16) and (17) reduce the solution of our problem to the determination of the shifted frequencies

$$\bar{k}_\ell = \bar{k}_\ell\left(k_0, k_1, \ldots; |\alpha_{01}|, |\alpha_{02}|, \ldots\right)$$

in terms of the unshifted frequencies and the coupling constants, as roots of the determinant or equations (4). This problem cannot be solved in all generality. We can, however, draw a few general conclusions from (16) and (17).

Due to the reflecting walls of our cavity of finite size, $D_{oo}(t)$ will be a complicated function of time. Even if the frequency levels of the empty cavity are equidistant, as we shall assume further on, (16) does not represent a periodic function, due to the level shift introduced by the atom, but rather a quasiperiodic phenomenon. If we choose, however, the dimensions of the cavity large compared to the

coherence length of the emitted wave train, we obtain conditions which approximate, during a certain time, the aperiodic emission in free space. The case of an atom radiating in free space is determined by (16) as a limiting process, letting our finite cavity become infinitely larger in all directions. This limiting process is, however, though uniquely determined by our procedure, a rather envolved operation. The difficulties encountered by previous theories were due to the fact that, considering only the limiting case of free space, they tried to determine the limiting value by guessing rather than by physical considerations.

We shall now assume a spherical cavity of radius R, large compared to the coherence wave length L. Then the unshifted frequencies will be equidistant,

$$k_r - k_{r-1} = \Delta k = \frac{\pi}{R}$$

and we shall assume the mechanical oscillator placed at the center of our sphere.

In order to find an approximate solution of the eigenvalue problem, we ask first whether or not we can restrict the ℓ-th vibration to two states only, one state of the field and the state of the excited mechanical oscillator, i.e. c_ℓ^ℓ and c_o^ℓ. In this case, we find immediately from (4)

$$\bar{k}_\ell = \frac{k_\ell + k_o}{2} + \sqrt{\left[\frac{k_\ell - k_o}{2}\right]^2 + |\alpha_{o\ell}|^2} \cong k_\ell + \frac{|\alpha_{o\ell}|^2}{k_\ell - k_o} \qquad (19)$$

However, before adopting (19), we have to make sure that in this case the neighboring frequencies $k_{\ell \pm 1}$ do not contribute appreciably to the collective motion. This is the case only if

$$\bar{k}_\ell - k_\ell \ll \Delta k \qquad (20)$$

Condition (20) can always be assured, even in the limit $R \to \infty$, at

sufficiently large distance from resonance

$$k_\ell - k_0 \gg |\alpha_{0\ell}|^2/\Delta k \cong \gamma \tag{21}$$

There exists, however, a domain

$$k_\ell - k_0 \leq |\alpha_{0\ell}|^2/\Delta k \cong \gamma \tag{22}$$

which determines the region of the natural line breadth.

In the resonance domain (22) the stationary vibrations of the total system are found to be collective, but this collective motion does not affect the total domain of the line breadth, but only a small fraction of it. In this case we have

$$\bar{k}_\ell - k_\ell \sim \Delta k \tag{23}$$

We find a first approximation of (16), if we forget for a moment about the resonance region (22) and introduce in (16) the asymptotic value (19). Neglecting small terms, we find

$$D_{00}(t) \cong \sum_\ell \frac{|\alpha_{0\ell}|^2 \exp(-i\bar{k}_\ell c t)}{(k_\ell - k_0)^2 + O(|\alpha_{0\ell}|^2/\Delta k^2)} \tag{24}$$

Putting

$$O(|\alpha_{0\ell}|^2/\Delta k^2) = \gamma_\ell^2$$

and assuming that in a sufficiently wide region of the spectrum the γ_ℓ do not depend on ℓ, $\gamma_\ell = \gamma$, we find in the limit $R \to \infty$ with $\bar{k} \to k_\ell$ the usual result of the older theories

$$D_{00}(t) \cong \frac{1}{\pi} \int_0^\infty \frac{\gamma \cdot \exp(-ikct)}{(k-k_0)^2 + \gamma^2}\, dk \cong \exp\left[-ik_0 ct - \gamma c|t|\right] \tag{25}$$

and, according to to (18), $t > 0$.

$$D_{ok}(t) \cong \frac{\alpha_{ko}}{k_k - k_o + i\gamma}\left\{\exp\left[-i(k_o - i\gamma)ct\right] - \exp\left[-ik_k ct\right]\right\} \quad (26)$$

It would be of considerable interest to find a rigorous solution of (16), which as we shall see later, will have a more complex structure than (25), but, so far, I have not succeeded in solving this problem.

5. The associated field. It is well known that quantum theory does not permit one to attribute to a quantum transition a finite, observable field. Only the quadratic expressions of the radiated field, such as energy and momentum are observables. Nevertheless we can, at least in the most important case in which only one photon is present in the field, introduce a corresponding classical field, which shall be called here the associated field, which is useful because it gives a direct though not completely rigorous picture of the space-time development of the quantum field. The associated field is defined in such a way that acting on an atom (test body), it produces the same matrix elements and effects as the non-diagonal quantum field*.

In order to construct, in our case, the associated field, we consider, in a sphere of sufficiently large radius R, the proper vibrations of the free field, limiting our attention, for our purpose, to electric dipole vibrations only, say in the z-direction, given by their respective Hertz vectors

$$Z_k = \sqrt{\frac{3hc}{2\pi k_k R}}\,\frac{\operatorname{Sen} k_k r}{k_k r}\exp\left(-ik_k ct\right) \quad (27)$$

This is normalized (asymptotically, i.e., for a sufficiently large sphere) in order to represent one photon of energy $k_k \cdot h/2\pi$, and

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* Since the concept of the associated field does not appear in the literature and seems not to be commonly known, it shall be discussed in more detail at another opportunity. To the present author it became known during discussions and common work with J. A. Balseiro, several years ago.

vanishes for r = R.

The coupling constants of (4) become in this case, for a harmonic mechanical oscillator of frequency k_0

$$\alpha_{0K} = \alpha_{K0} = \sqrt{\frac{3}{2}\frac{a}{R} k_0 k_K} \tag{28}$$

where $a = e^2 / mc^2$ is the classical electron radius. They have a simple physical meaning and represent the Fourier coefficients of the electric moment distribution in the emitting mechanical system during the quantum transition.

We define, now, the field associated with our emission process by

$$Z_{ass} = \sum_{k,\ell} \frac{k_k}{\bar{k}_\ell} Z_{0k}^{\ell} \tag{29}$$

with

$$Z_{rk}^{\ell} = C_r^{\ell *} \cdot c_k^{\ell} \cdot Z_k \cdot \exp\left(i \cdot (k_k - \bar{k}_\ell)\, ct\right) \tag{30}$$

The physical meaning of (30) is immediately clear: it represents for the r-th wave packet, the intensity with which the k-th vibration of the free field contributes to the ℓ-th proper vibration of the system, with the common frequency $\bar{k}_\ell$.

The factor $k_k / \bar{k}_\ell$ in (29) is due to the fact that we have to consider not the Hertz vectors, but rather the potentials of the different free vibrations to be additive. In our case (r = 0) we can use with good approximation

$$k_k / \bar{k}_\ell = k_k / (k_0 - i\gamma)$$

as long as we deal with conditions which do not differ sensibly from the classical value (2).

The coefficients of (30), $c_r^{\ell *} \cdot c_k^{\ell}$ are the probability amplitudes for finding the k-th photon with the ℓ-th frequency. It fol-

lows immediately from our construction, that these coefficients are square integrable. The value of the square integral of the coefficients of (29) is smaller than unity, because it does not contain the configuration in which the mechanical system is excited and no field is present. The square integrability of the coefficients assures that the spectrum of (29) is a proper spectrum, contrary to the spectrum of (2). This proves, at the same time, that the classical expression (1) cannot be correct and differs from (29).

We shall now examine in more detail the associated field (29). Making use of relations (30), (27), (14) and (15) we find

$$Z_{ass} = \sum_{\ell, K \neq 0} \frac{\alpha_{K0}}{\bar{k}_\ell - k_K} \left(1 + \sum_r \frac{\alpha_{or}\alpha_{ro}}{(\bar{k}_\ell - k_K)^2} \right)^{-1} \sqrt{\frac{3hc}{2\pi k_K R}} \times \frac{1}{k_0 - i\gamma} \frac{\sin k_K r}{r} \exp(-i\bar{k}_\ell c t) \tag{31}$$

The double sum (31) corresponds closely to the double integral (2), without containing, however, any divergent term.

We mention here, without giving the proof explicitly, that the associate field (31) obeys Maxwell's equations for free space, outside the charge and current distributions of the emitting atoms [2].

We shall show now that in the approximation given in N° 4, (31) leads back to the classical expression (1). Using (26), the summation over ℓ can immediately be carried through and leads to

$$Z_{ass} = \sum_{K \neq 0} \frac{\alpha_{K0}}{k_K - k_0 + i\gamma} \sqrt{\frac{3hc}{2\pi k_K R}} \cdot \frac{1}{k_0 - i\gamma} \frac{\sin k_K r}{r} \times \left\{ \exp[-i(k_0 - i\gamma)ct - \exp(-ik_K ct) \right\} \tag{32}$$

which, transformed into an integral, is essentially equivalent to (1).

It is more instructive, however, to carry out, in (31) first the summation over K, observing (28)

$$\sum \sqrt{\frac{9hc\alpha}{4\pi R^2} k_0} \cdot \frac{1}{\bar{k}_\ell - k_K} \frac{1}{k_0 - i\gamma} \frac{\sin k_K r}{r}$$

This summation corresponds to the integration over the distribution (3) in (2). Starting from the identity

$$\frac{1}{\sin \bar{k} R} \frac{\sin \bar{k}(r-R)}{r} = \sum_{K \neq 0} \frac{1}{R} \left\{ \frac{1}{\bar{k} - k_K} - \frac{1}{\bar{k} + k_K} \right\} \frac{\sin k_K r}{r} \qquad (33)$$

which can easily be verified by Fourier development, we obtain, omitting the negligible second term on the right hand side of (33)

$$\sum_{K \neq 0} \frac{1}{R} \frac{1}{\bar{k}_\ell - k_K} \frac{\sin k_K r}{r} \cong \frac{\sin \bar{k}_\ell (r-R)}{r \cdot \sin \bar{k}_\ell R} \qquad (34)$$

This differs essentially from the result which we would obtain by using the distribution (3) or any part of it. The main difference consists in the appearance of the phase

$$\delta_\ell = \bar{k}_\ell R \equiv \pm (\bar{k}_\ell - k_\ell) \cdot R$$

which does not appear in the distribution (3) and which tends to a finite value, even in the limit $R \longrightarrow \infty$.

6. The rigorous treatment of the problem of field propagation.

We shall now turn back to the rigorous formulation of our theory. The inconsistencies, which we have found in N° 5 are essentially due to an inconsistency in the underlying assumptions. In order to compare our theory with previous ones, we had necessarily to

refer to classical field concepts, outside of their proper domain of applicability. We have seen how the emission process depends on the coupling between the source and the field. What we have omitted in constructing our associated field is the fact, that the same mechanism which determines the excitation of the field by the source, is essential also, as soon as we want to observe the emitted field by means of a real test body, i.e., by a second oscillator or atom.

In order to obtain a consistent treatment of the fundamental problem of field propagation in space and time, we have, therefore, to couple the field vibrations with two mechanical oscillators, placed at a certain distance from each other, the one excited (source) and the other in the ground state (test body). In order to describe this initial configuration, we have to determine first, as in N° 2, the proper vibrations of the total coupled system and to construct afterwards, a wave packet, which represents the initial configuration. The time development of this wave packet determines, then, what is accessible to observation, i.e., the excitation in time of the test body, as a function of time and the relative distance between source and test body. Finer details of the problem of field propagation can be obtained only in this way. We can already see from our previous considerations, that these details will be different from the ones given by classical theory and cannot be expressed any longer by means of the usual classical concepts.

The detailed study of these problems requires, however, the development of new mathematical methods and shall not be attempted in the present paper.

7. Conclusions. We have seen above, that quantum theory permits us to formulate the problem of the emission process during a so-called quantum transition in an unambiguous way which leads only in first approximation to the classical expressions. So far, we have not been able to obtain explicit expressions for the higher approximations and new methods will have to be developed in order to solve equation

(16) and the corresponding problem of Nº 6.

Still, we can already conclude that the classical expressions (1) and (2) cannot be valid rigorously. The field emitted during a quantum transition can certainly not be represented by a single pole in the complex plane. There exist, therefore, in the domain of the natural line breadth, new and observable physical phenomena, which are not accounted for by classical theory. One phenomenon in this sense was observed several years ago [3] and has, as a matter of fact, conduced to the present theory. It is not impossible that the phenomenon observed by Lennuier will be found included in the higher order approximations of the present theory. It would be desirable that this phenomenon be verified by other, independent experiments.

From the formal point of view, a main result of the present theory is that it shows at least in one easily accessible special case, that there is no room in physics for improper functions or distributions. Quantum electrodynamics uses improper functions as essential elements. They will have to be removed one by one, using physical arguments for finding the corresponding finite expressions. The present theory may be helpful in other cases for finding these expressions.

The most important conclusion of the present theory, however, is the fact that a quantum theory of energy transfer between distant systems has to revise even the apparently simple problem of field propagation in space and time, beyond the limits of classical concepts.

[1] C. R. 236, 465 (1953).

[2] Strictly speaking the above statement is valid only approximately, neglecting terms of the order of the contribution of negative frequencies. Soc: G. Beck Ciencia e Investigación, 6, 573 (1950).

[3] R. Lennuier, Ann. de Phys. 2, 233 (1947).